SEPTEMBER 2023, ISSUE 122

WELCOME

People have been trying to capture lightning in a bottle for nearly three centuries. Fifty years after Benjamin Franklin's famous experiment with a kite and a Leyden jar, Alessandro Volta did just that, creating the first continuous and stable source of electric current: the voltaic cell, or battery.

Batteries have been part of everyday life for a long time. Those of us of a certain age will groan when we remember the phrase "batteries not included," usually associated with gifts that wouldn't work out of the box unless we could scrounge up the correct-sized batteries from a cabinet or drawer. More recently, many of our devices use rechargeable cells, but even those aren't perfect. After months or years of use, their charging capacity decreases or their ability to hold a charge for more than a few hours deteriorates.

In this issue of *The Bridge*, we are focusing on battery research, which encompasses many scientific fields and analytical methods. What is going on at an atomic level when a battery is charged and when it discharges? How do the molecular species change? How does the internal structure of the battery itself change during these processes? What are the energetics of charging and discharging?

So many questions that a consumer rarely needs to think about but that the people who are developing the next generations of batteries must consider. They are very expensive components of certain devices—cars, for example—so making sure their replacement cycle is acceptable and that we know what to do with batteries after they are retired are important considerations. We rely on our cell phone and laptop batteries to keep us connected when we aren't tethered to a wall outlet. People's lives are at stake when they rely on embedded devices powered by batteries. And we don't want batteries to overheat while being charged or in use.

Read on to learn more about Rigaku's involvement in battery research, including links to past and upcoming webinars, podcasts, *Rigaku Journal* articles and application notes.

BATTERY IN SPOTLIGHT

Discover our advanced instrumentation solutions tailored for battery research. From investigation of new battery materials to quality control, we provide the tools researchers need to validate materials and optimize energy storage for higher efficiency and energy density.

Rigaku offers a variety of instruments designed for battery research, including:

1. X-ray Diffraction (XRD): These instruments are crucial for analyzing the crystallographic structure of materials, which is essential for understanding their properties in battery applications.
2. X-ray Fluorescence (XRF): XRF spectrometers help in elemental analysis, ensuring the quality and composition of materials used in batteries.
3. X-ray computed tomography (CT): This is a technique to image objects in 3D non-destructively. X-ray CT is effective for failure analysis of multilayered battery cells used for battery products without disassembling them.
4. Small-angle X-ray scattering (SAXS): This technique can determine nano-particle size distributions, resolve the size and shape of (mono-disperse) macro-molecules, determine pore sizes, characteristic distances of partially ordered materials, and much more.

Check our website at http://battery.rigaku.com/ to discover Rigaku solutions for battery analysis.

Learn More

> WEBINAR SERIES

BENEATH THE SURFACE: X-RAY ANALYSES OF BATTERY MATERIALS AND STRUCTURES

Are you facing challenges, such as cost, material shortages, and safety issues, in your battery research, recycling, or process control? In-depth analysis of chemical composition of raw materials, in operando monitoring of crystal structures at an atomic and molecular level during charging and discharging, and even non-destructive imaging of assembled batteries can provide insights that help you overcome various challenges.

In this webinar series, you will learn how to leverage X-ray analysis techniques to gain insights into battery performance. We will cover X-ray diffraction (XRD), X-ray fluorescence (XRF) elemental analysis, and X-ray computed tomography (CT) non-destructive testing.

Our expert speakers will guide you through experimental setups and real-world applications. Whether you're a researcher, engineer, or process control manager, this series will empower you with the knowledge to understand battery behavior at a nanometer to millimeter scale. You can register for individual episodes.

Watch the first episode of the series

> UPCOMING BATTERY WEBINARS

HOW TO RUN IN OPERANDO XRD EXPERIMENTS
Date/time: Wednesday, November 15, 2023 01:00 PM CDT
Presenter: Keisuke Saito, PhD | Co-presenter: Tim Bradow | Host: Aya Takase

Learn More

PAIR DISTRIBUTION FUNCTION (PDF) ANALYSIS FOR EVERYDAY BATTERY ANALYSIS
Date/time: Wednesday, February 21, 2024 01:00 PM CDT
Presenter: Simon Bates | Co-presenter: Tim Bradow | Host: Aya Takase

Learn More

NON-DESTRUCTIVE ELEMENTAL ANALYSIS OF BATTERIES USING XRF
Date/time: Wednesday, June 19, 2024 01:00 PM CDT
Presenter: Amber Quevy | Co-presenter: Tim Bradow | Host: Aya Takase

Learn More

NON-DESTRUCTIVE INSPECTION OF BATTERIES USING X-RAY COMPUTED TOMOGRAPHY
Date/time: Wednesday, August 21, 2024 01:00 PM CDT
Presenter: Angela Criswell | Co-presenter: Tim Bradow | Host: Aya Takase

Learn More

> BATTERY TOPICS IN RIGAKU JOURNAL

Utilization of X-ray diffraction data in machine-learning based material exploration for all-solid-state lithium batteries

Many researchers have been developing and analyzing potential electrode materials and solid electrolytes, with a particular focus on crystalline materials. All-solid-state lithium batteries would give rise to the possibility of all battery components being made from crystalline materials; therefore, the importance of phase identification and crystal structure analyses by X-ray diffraction (XRD) measurements will increase. In this technical note, we will introduce XRD measurements and explore how the data can be used in the search for materials related to all-solid-state batteries, along with examples of our own research.
>Read full article

Chemical State Analysis by X-Ray Emission Spectroscopy
We are evaluating the applicability of Si-based negative electrode materials and next-generation battery materials for lithium-ion batteries using double-crystal spectroscopy with high-energy resolution. Quantitative analysis results of Li–Si alloy composition and side reaction products were reported based on changes in the Si Kβ spectral profile during electrochemical charging and discharging. It is known that the X-ray emission spectrum changes depending on the chemical state of the material, but the technique is not actively applied to chemical state analysis currently. In this paper, as the basis for describing the X-ray emission analysis method, we explain the optical system required to obtain high resolution, describe the interpretation of the X-ray emission spectrum and spectral changes due to the chemical state, and introduce application examples.
>Read full article

Characterization of lithium-ion battery materials with SmartLab
To examine the crystallization and phase ID analysis of synthesized battery materials, lab-scale X-ray diffractometers that are readily available for research are frequently used. On the other hand, operando (or in-situ) measurement of the changes in the crystal structure of the positive and negative electrode materials during the charging and discharging processes are frequently conducted at synchrotron facilities where high-intensity X-rays are available. Recently, operando measurement has become possible even with lab-scale X-ray diffractometers due to improved performance of X-ray sources, optical elements, and detectors. This article introduces examples of characterizing lithium-ion battery materials using SmartLab.
>Read full article

> A new publication from Rigaku's X-ray Research Lab

Crystallization process of Li_3PS_4 investigated by X-ray total scattering measurement and the reverse Monte Carlo method
All-solid-state Li-ion batteries (LIBs) are scoped to large-scale energy storage/conversion applications such as electric vehicles and smart grids storing solar energy because of their potential, high energy density and high cycling characteristics. Solid electrolytes are a key component of all-solid-state LIBs. The binary system xLi_2S $(100-x)P_2S_5$ ($0 \le x \le 100$, mol%) is one candidate for all-solid-state LIBs due to relatively high electrochemical stability because they contain no heavy metallic elements. We evaluated the local structure of $75Li_2S$ $25P_2S_5$ (mol%) Li_3PS_4 glass with a structural phase transition from glass to crystal between 298 K and 523 K by X-ray total scattering data coupled with Reverse Monte Carlo (RMC) modeling. The RMC results suggest the PS_4 anion remains a tetrahedron over the wide range from glass to crystal, and that PS_4 libration plays an important role in Li-ion migration in Li_3PS_4 solid electrolytes.
>Read full article

> BATTERY IN THE NEWS

September 6, 2023: Scientists at Argonne National Laboratory discovered a previously unknown reaction mechanism that reveals the reason for the short lifetimes of lithium-sulfur batteries. Scaled up to commercial size, these batteries, which have several advantages over lithium-ion batteries, show a rapid decline in performance with repeated charge and discharge.

September 11, 2023: Scientists from the University of Cincinnati have created a redox-flow battery that could lead to more environmentally friendly energy solutions. This battery eliminates the expensive and relatively inefficient membrane found in conventional designs. This development is particularly significant for optimizing the extensive energy storage needs of wind and solar farms.

September 13, 2023: By examining X-ray images, researchers at MIT, Stanford University, SLAC National Accelerator, and the Toyota Research Institute have observed how lithium ions flow through a battery interface, which could help engineers optimize the lithium iron phosphate material's design.

September 21, 2023: Scientists from Dalhousie University published the results of experiments that improve lithium-ion cells by replacing polyethylene terephthalate (PET) tape with more chemically stable polypropylene and polyimide (Kapton). PET tape can depolymerize in the absence of effective electrolyte additives, which can induce substantial self-discharge in a lithium-ion cell.

Battery Flyer
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Battery App Notes
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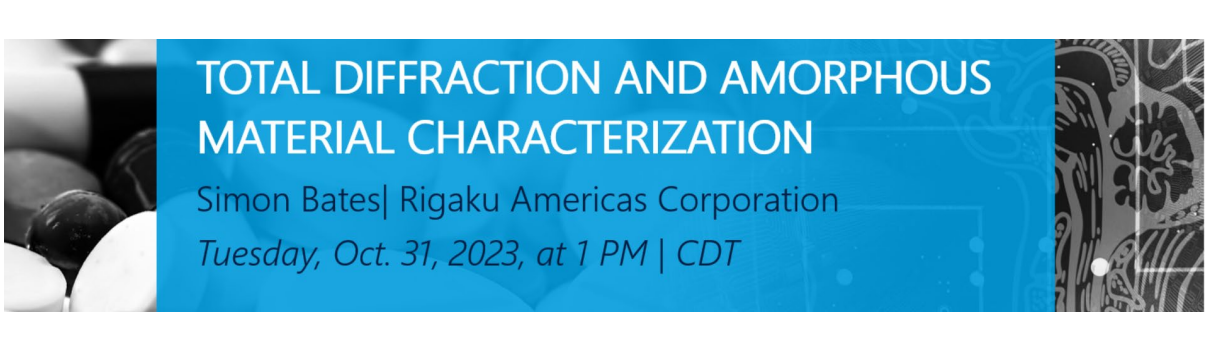
Joint Battery Webinar with Micromeritics
Watch

Joint Battery Webinar with Retsch
Watch

The Battery Lab is a podcast empowering the researchers powering the future. Every episode features insights from the industry experts, leading academics and cutting-edge research advancing batteries — and society — to the next level of safety and efficiency. From raw materials to analysis to state-of-the-art designs, if you care about fueling the future, you've come to the right place. Welcome to the Battery Lab!
Listen to the Podcast >

RIGAKU WEBINARS



Date/time
Tuesday, October 31, 2023, at 1 PM | CDT
Host: Simon Bates, Rigaku Americas Corporation

X-ray powder diffraction is regarded as the gold standard with respect to the characterization of crystalline solid forms in pharmaceutical materials. However, the traditional Bragg peak crystalline methods become less relevant with the general trends of the increasing complexity of active molecules and the prevalence of non-crystalline forms (amorphous, meso-phasic, nano-phases, etc.).

In this presentation, I will discuss:

- Some of the latest X-ray Total Diffraction approaches using laboratory equipment can provide enhanced analytical capabilities more suited to modern pharmaceutics.
- Total Diffraction approaches exhibit greater similarity to Chemometrics and pattern recognition than traditional X-ray diffraction analysis.

Register

Date/time
Wednesday, November 15, 2023, Session 1: at 9AM and Session 2: at 4PM | CET
Host: Carmen Kaiser-Bruegmann, XRF Application Scientist, Rigaku Europe SE

Join us for our free 45-minute webinar on XRF, the leading analytical technique in many fields. Discover how to improve material quality testing through proper sample preparation, addressing issues such as sample in homogeneity and error.

Highlights include:

- Learn about the fusion method, eliminating sample matrix and mineralogical challenges.
- Gain insight into a calibration method for different elements.
- Understand the benefits of fusion: error reduction, matrix dilution, synthetic standards and broad oxide calibration.
- Improve analytical accuracy and expand your applications.
- Meet Rigaku's XRF specialist for practical guidance on fusion method development and analysis.
- Get answers during the Q&A session.

Don't miss this opportunity to enhance your materials analysis capabilities. After the webinar, you'll receive a free, comprehensive download package.

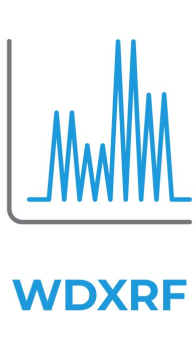
Register

FEATURED APPLICATION NOTES

EDXRF

Phosphorus on Fabric
Applied Rigaku Technologies

Clothing fabrics for work clothes, uniforms, baby clothing and other uses can be coated with a phosphorus compound for the purpose of flame retardancy. Bromine and antimony are typically no longer used in clothing due to the toxicity of these heavier elements, but can still be used in heavier textiles such as draperies, carpet and mattress materials. During the coating and processing of treated fabrics, the flame retardant material must be closely monitored to ensure optimum quality without incurring cost overruns due to product rejection or overuse of chemicals. EDXRF is an excellent measurement method. Quick and simple, EDXRF offers QC technicians a reliable means of monitoring flame retardant concentrations throughout the entire QC process. The analysis of phosphorus flame retardant compound on fabric is demonstrated.
Read More >



WDXRF

Quality and Process Control Analysis of Natural and Processed Iron Ores by the Pressed Powder Method
Rigaku Corporation

Iron ore is the most abundant mineral resources and is also one of the most important materials in modern industries. Since the amount and cost of seaborne trade have increased in recent years, analytical requirements are becoming more stringent. Total iron (T.Fe) concentration in iron ore is a focal point for trade. Therefore, analysis to determine total iron requires high accuracy.

Since iron ore has complex matrices owing to varied mineral composition, appropriate corrections for these matrix effects are required in XRF analysis. The conventional correction technique for total iron is a method using Compton scattering as an internal standard, but it has not been rigorous enough to meet the requirements of the iron ore industry. Rigaku has developed an improved Compton scattering method by integrating theoretical alpha corrections to significantly improve analytical results. This note demonstrates an improved method to determine total iron in natural and processed iron ores by the pressed powder method.
Read more >

PODCASTS

Understanding Semiconductors: Modern Metrology from Lab to Fab, is a podcast for engineering leaders in characterization, metrology, process, and analytics, looking for discussion around semiconductor metrology challenges. Each episode will feature a conversation with technology experts about problems facing the semiconductor metrology industry.
Listen to New Episodes >

The Opioid Matrix is a podcast for anyone looking for the latest information in the illegal drug supply chain—beginning to end. Each episode will feature a discussion with industry experts about the current opioid crisis, including drug trafficking, drug manufacturing, drug identification, drug addiction, as well as the role of government, law enforcement, new health and social programs, and more.
Listen to New Episodes >

The Pharma Lab Show is a podcast exploring the technologies, analysis, and innovation that goes into bringing the pharmaceuticals that allow humanity to live longer, fuller, healthier lives.

Each episode features interviews with industry leaders and experts who share how they are working tirelessly to bring these life-changing products into the world.
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